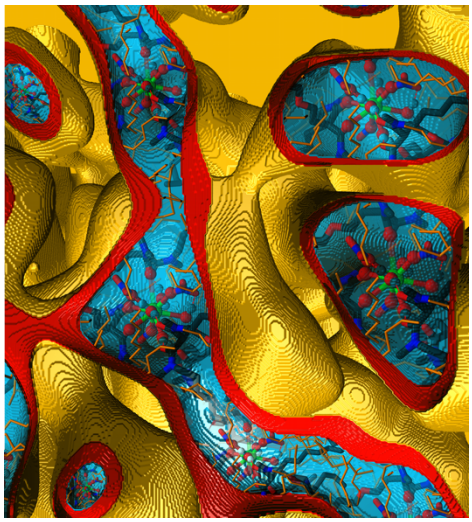
Open Postdoctoral position at
Institut de Chimie Séparative de Marcoule (ICSM), Bagnols-sur-Cèze, France

Modeling of liquid-liquid extraction by a microemulsion model

Position for 12 months (renewable) – Starting date: April 2023



Credit: M. Duvail / ICSM

In the context of recycling strategic metals, and in particular rare-earths, **liquid-liquid extraction** remains the essential separation method. **The modeling of this process** is of paramount importance as it is the only way to understand quantitatively the different effects and mechanisms involved[1]. In this context several techniques are possible. Work at the molecular scale has shown how complexation and organisation take place, but the systems formed are large in size with an organisation similar to that of **microemulsions**, which makes **modelling at larger scales**, and in particular at the **mesoscopic scale**, necessary.

The computational approach will consist in **simulating the formation of aggregates** composed of lanthanide salts in presence of extractant molecules in an organic solvent. The idea is to develop a **code predicting the thermodynamics** of these processes from a microemulsion model adapted to liquid-liquid extraction[2]. This work will be based on molecular dynamics simulations[3] and experimental measurements to parametrize the model. Particular attention will be paid to the **curvature effects** that control the size of the species formed in solution, the **role of co-extracted anions** in modifying selectivity, as well as the different ways to model the role of **complexation**.

The objectives of this project will provide insights into the **understanding of solvent extraction** which is one of the most widespread recycling methods for metals. The originality consists of **coupling concepts of molecular chemistry** for the short-range effects **to soft matter theory** (microemulsion) in order to propose a self-consistent description of solvent extraction. The practical application of this method to the recycling of metals of interest aims to improve and propose more efficient and resource-saving processes.

Profile: Eligible candidates should have a good knowledge of physical chemistry or chemical physics. Good knowledge of programming is also important because of the modeling aspect of the project. Good oral and written communication and teamwork skills are also essential, as the candidate should collaborate with a team of experimental researchers.

Funding: The postdoc position is funded by the University of Montpellier within the ANR MULTISEPAR project. The duration of the contract is 18 months.

Net salary: ~ 2000 € / month

Further information: The successful candidate will join the LMCT group of ICSM. A position of assistant professor (maître de conférence) is planned next year in the laboratory on this theme.

Contact: To apply, please send a cover letter, a detailed CV, and references to Pr. Jean-François Dufrêche (jean-francois.dufreche@icsm.fr) and Dr. Magali Duvail (magali.duvail@cea.fr).

Mesoscopic Modelling and Theoretical Chemistry Group (LMCT)
ICSM UMR 5257 – BP 17171
Site de Marcoule
F-30207 Bagnols sur Cèze, France

http://www.icsm.fr/icsm_engl/lmct_en.html

[1] M. Spadina *et al.*, **ACS Nano** *13*, 3745 (2019). DOI: 10.1021/acsnano.9b07605
[2] S. Gourdin-Bertin *et al.*, **Solv. Extr. Ion Exch.** *40*, 28 (2022). DOI: 10.1080/07366299.2021.1953259
[3] S. Stemplinger *et al.*, **J. Mol. Liq.** *348*, 118035 (2022). DOI: 10.1016/j.molliq.2021.118035